

1,4-Dioxane
123-91-1 | DTXSID4020533

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 11.2 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.65e-01

Confidence level: 8.64e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Dioxane

Measured: 11.4

Predicted: 11.2

Image not found

dl-Diepoxbutane

Measured: 11.6

Predicted: 9.80

Image not found

2,2'-Bioxirane

Measured: 11.6

Predicted: 9.80

Image not found

1,3-Dioxolane

Measured: 13.5

Predicted: 11.9

Image not found

Ethylene glycol dimethyl ether

Measured: 11.1

Predicted: 10.9

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2-Methyl-1,3-dioxolane

Measured: 7.57

Predicted: 7.35